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Computer modeling of multiphase fluid flow (in fractured and porous media)

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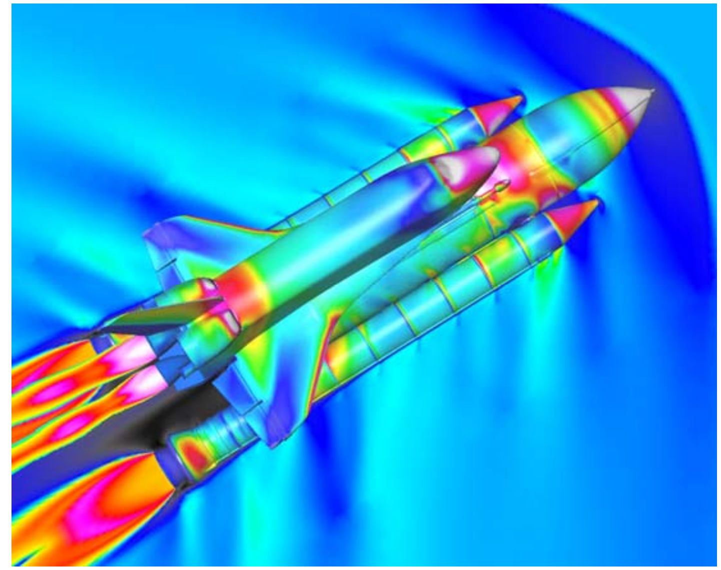
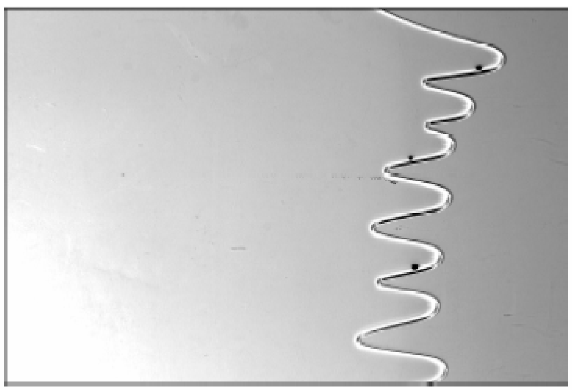
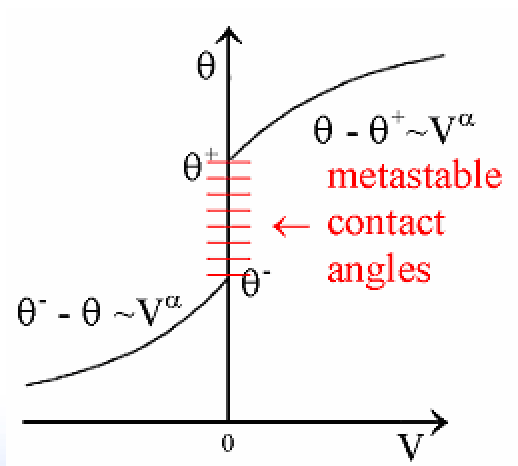


Two computational challenges:

1. Complex interface dynamics (topological changes)
2. Complex contact line dynamics



Veretennikov *et al*. 2005



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Research Strategy

- Integrated computer modeling and experiments (but will discuss only simulations today)
- Develop a suite of computer modeling methods with complementary strengths and weaknesses
- Particle-based methods:
- Lattice Boltzmann (LB)
- Smoothed particle hydrodynamics (SPH)
- Dissipative particle dynamics (DPD)
- Grid-based Navier Stokes solvers with interface tracking/capturing

- Level set interface tracking (LS)
- Volume of fluid interface tracing (VOF)

} Use indicator function that is advected with flow

Particle-based vs. grid-based models for multiphase fluid flow

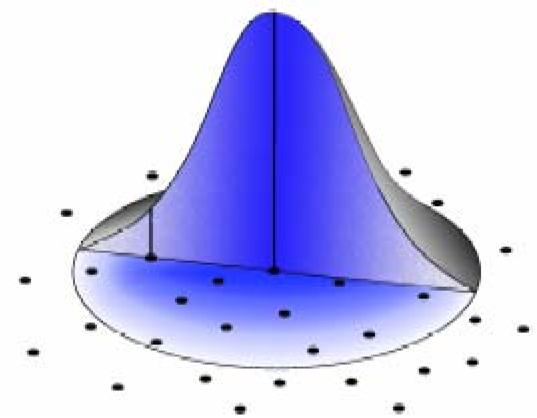
❖ Advantages:

- Particles move with fluid (no interface tracking required)
- Rigorous mass conservation
- Reproduce complex behaviors associated with fluid-fluid-solid interface dynamics
- Relatively simple code
- Relatively easy to add additional physics

❖ Disadvantages:

- Less (sometimes much less) computationally efficient than grid-based Navier Stokes solvers.
- Fundamental fluid properties must be measured – they are controlled by particle-particle interactions

Smoothed particle hydrodynamics



- Continuous fields are represented by sum of weighting functions centered on particles:

  $f(x) = \Sigma m_i f_i W(|\mathbf{x} - \mathbf{x}_i|)/\rho_i$, $\rho(x) = \Sigma m_i W(|\mathbf{x} - \mathbf{x}_i|)$

  $\nabla f(x) = \Sigma m_i f_i \nabla W(|\mathbf{x} - \mathbf{x}_i|)/\rho_i$

- Conservation equations:

  $d\mathbf{V}/dt = \nabla \cdot P/\rho$, $d\rho/dt = \rho\nabla \cdot \mathbf{V}$ (or calculate density from particle positions via weighting function).

- Calculate pressure from density via equation of state.
- Approximate derivatives using weighting functions (compare with finite difference).
- $d\mathbf{V}/dt + \; = -\nabla P/\rho + \eta \nabla^2 \mathbf{V} + F_{ex}$ (Navier Stokes equation)
- $d\mathbf{V}_i/dt = \Sigma m_i (P_i/\rho_i^2 + P_j/\rho_j^2) \cdot \nabla W(|\mathbf{x} - \mathbf{x}_i|)/\rho_i$ +
- additional terms to represent effects of viscosity, interactions with solid surfaces, surface tension ....

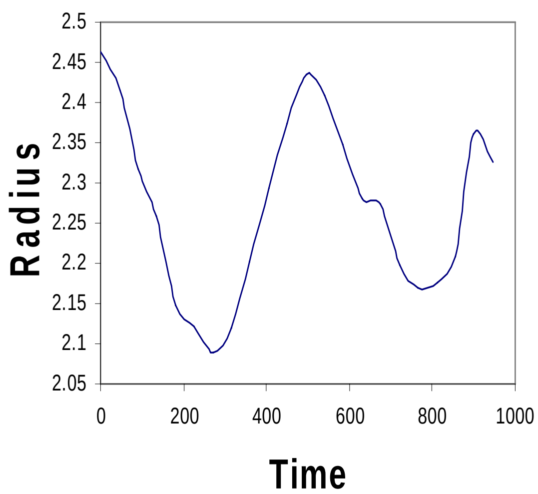
Smoothed particle hydrodynamics: Advantages and disadvantages

- Versatile - can be used to simulate fluids and solids under extreme conditions.
- Numerically unstable under some conditions (we have had no problems).
- Most applications have been in astrophysical fluid dynamics.
- Simulates continuum equations, but particle—particle interactions can be added to simulate phase separation, surface tension, wetting etc.
- Insufficient theoretical basis for these ‘hybrid models’.
- Galilean invariant (forces depend only on position and velocity differences).
- Intrinsic (particle based) contribution to fluid properties (model fluid properties are not the same as those used in the ‘governing’ equations.

Estimation of surface tension

$\sigma = 0.18 \pm 5\%$

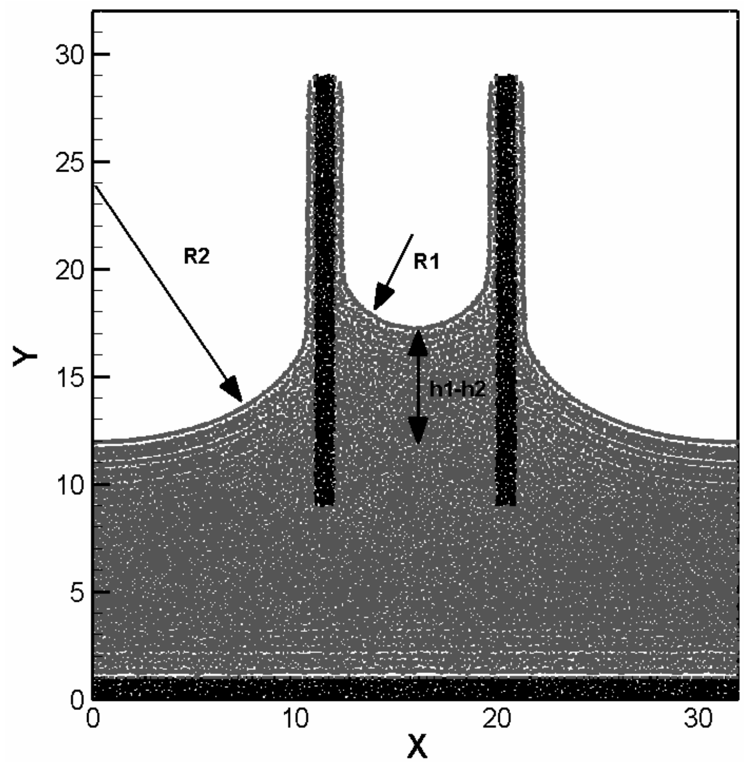
Bubble oscillation



period of oscillation

$$\tau = 2\pi\sqrt{\frac{R^3\rho}{6\sigma}}$$

Capillary rise



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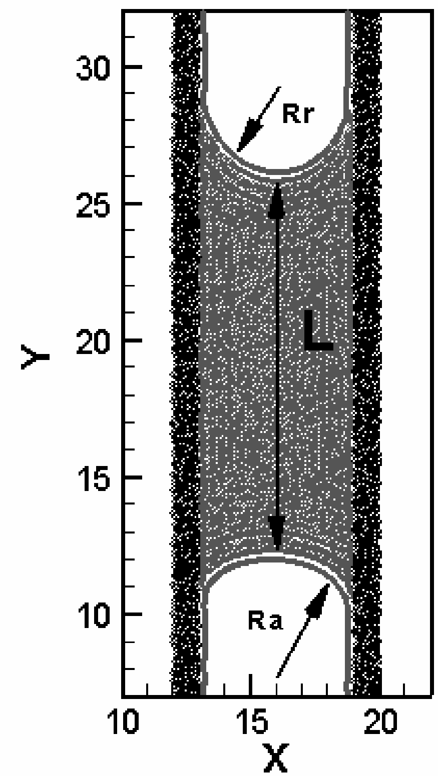
$$\rho g\left(h_1 - h_2\right) = \sigma\left(\frac{1}{R_1} - \frac{1}{R_2}\right)$$

Droplet in fracture

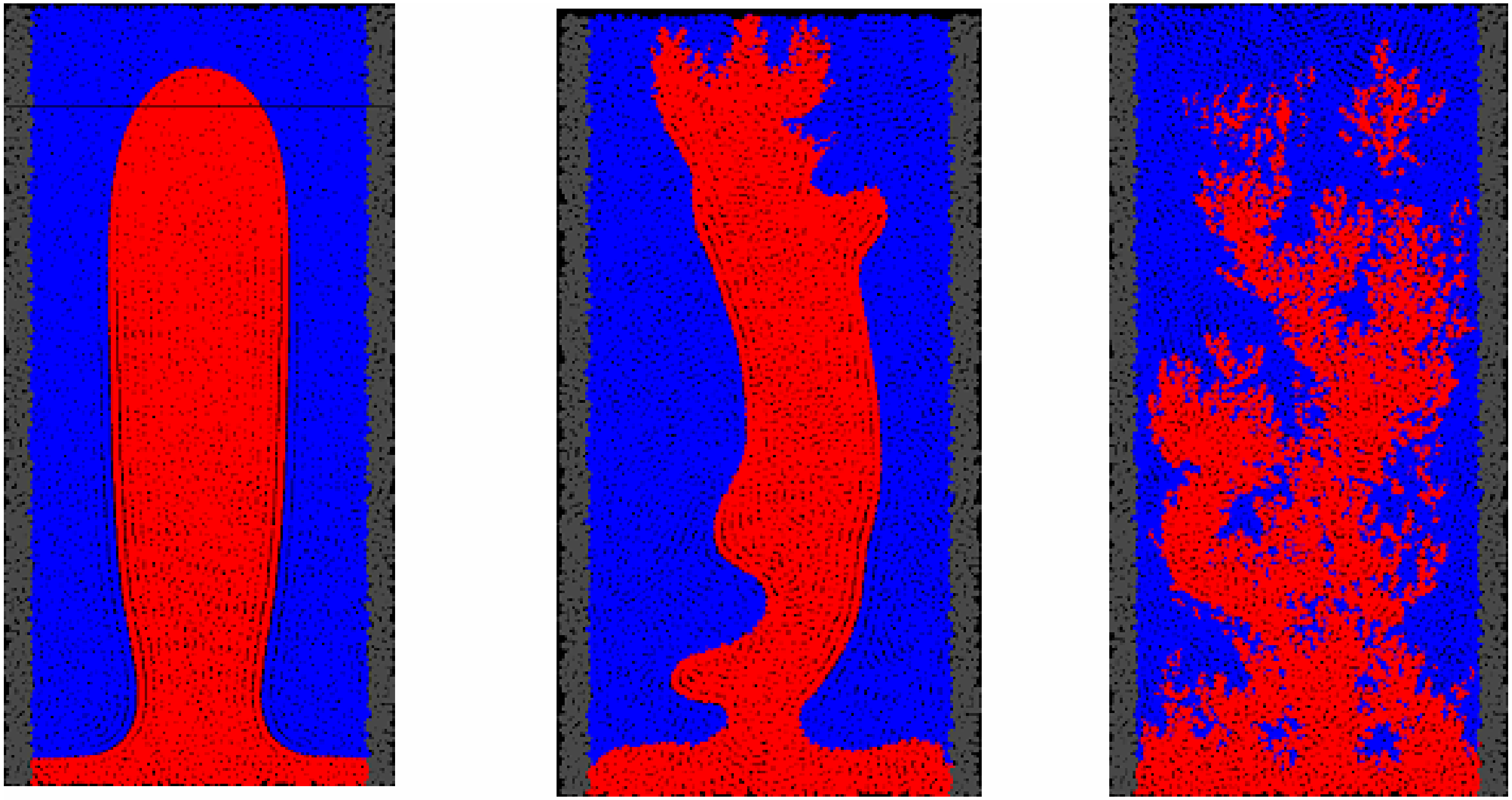


$$\mathrm{v} = \frac{b^2}{12\mu}\left\{\rho g + \frac{\sigma}{L}\left(\frac{1}{R_a} - \frac{1}{R_r}\right)\right\}$$

Physical Review E: in press

Also dependence of internal pressure on bubble radius

Smoothed particle hydrodynamics simulation of viscous fingers



$Ca = 0.316$ $Ca = 5.31$ $Ca = \infty$

$m_k = 1$, $m_l = 0.2$, $\mu_k = 1$ and $\mu_l = 16$. $Ca = \mu U/\Gamma$

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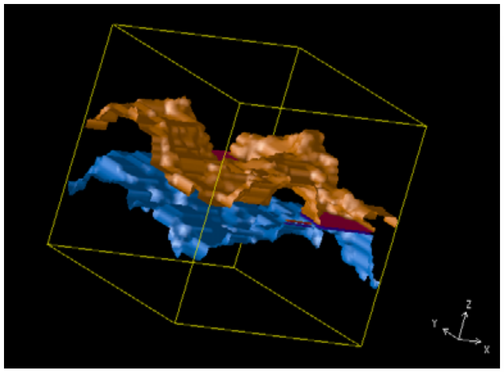
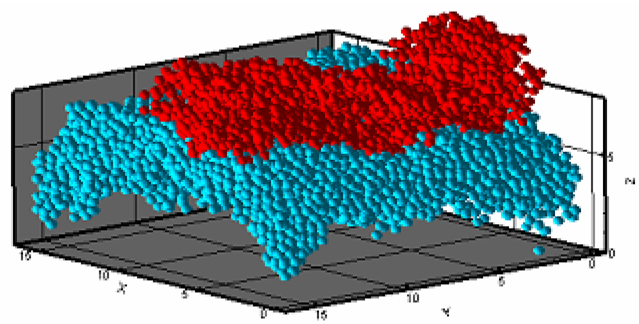
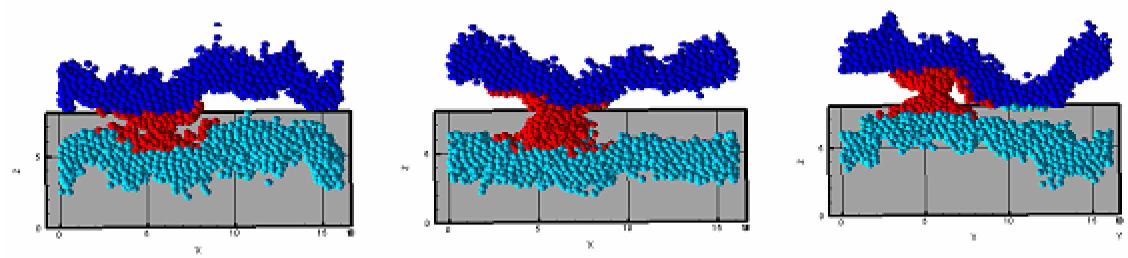
Smoothes particle hydrodynamics simulation of precipitate growth in a fracture aperture





a)

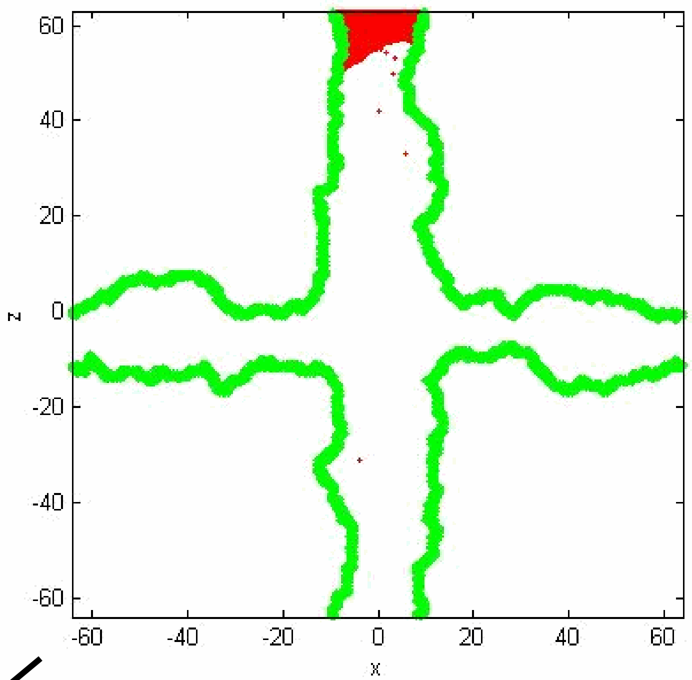


b) y = 4 *c) y* = 8 *d) y* = 12

Dissipative particle dynamics: Advantages and disadvantages.

- Very versatile: can handle complex fluids and complex boundary conditions.
- Numerically stable: Dissipative and random forces act as thermostat, and deviation of kinetic temperature from fluctuation-dissipation temperature can be used to determine acceptable step size.
- Not very computationally efficient – but much better than MD.
- Soft potential $\Rightarrow$ high compressibility.
- Includes effects of thermal fluctuations.
- Must measure model parameters – like MD.
- Galilean invariant (forces depend only on position and velocity differences)

Dissipative particle dynamics simulation of penetration of fluid into a fracture junction



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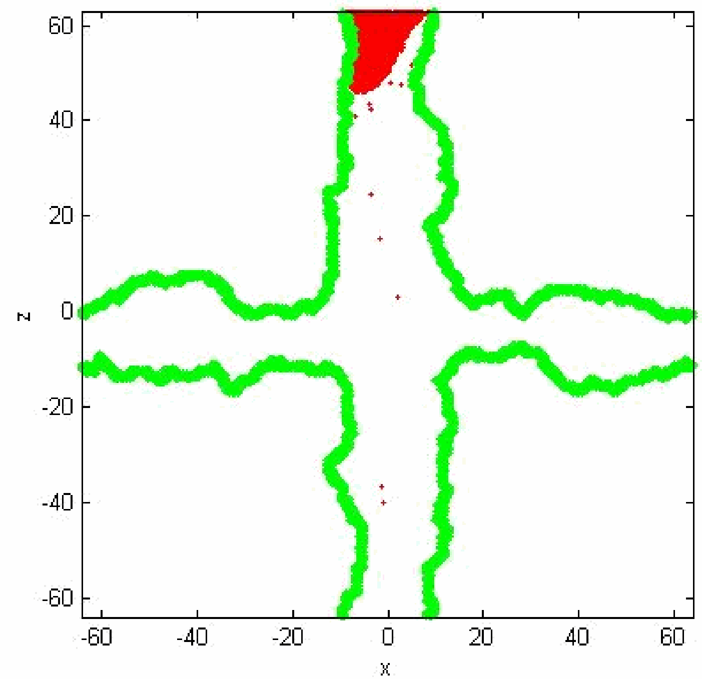
Strongly wetting



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Weakly wetting

Dissipative particle dynamics

- Particles interact through conservative, dissipative and random forcers
- Conservative particle-particles are soft – large time steps
- Individual particles represent (very) small fluid volumes
- Interactions rigorously conserve momentum
- Fluctuation-dissipation relationship between random and dissipative interactions
- Algorithm is like thermostatted molecular dynamics
- Short range repulsive + long(er) range attractive interactions lead to phase separation

Navier Stokes solvers with indicator function interface capturing

- Numerical solution of Navier Stokes equation.
- Conservation of material: $\nabla \bullet \mathbf{V} = 0$
- Conservation of momentum:

  $\rho d\mathbf{V}/dt = -\rho (\mathbf{V} \bullet \nabla)\mathbf{V} - \nabla P + \eta \nabla^2 \mathbf{V} + \mathbf{F}_{ex}$
- Level set interface capturing: Fluid-fluid interface is the 'level-set' (zero level cut) of the level set function, $\phi(\mathbf{x})$, which is advected with the flow.
- Volume of fluid interface tracking: The indicator function, $\phi(\mathbf{x})$, which is advected with the flow, has a value of 1 in fluid 1, a value of 0 in fluid 2, and and $0<F<1$ for grid cells that contain part of the fluid-fluid interface.

Simulation of dripping fauces: Complex chaotic dynamics (deterministic chaos)

Three-dimensional (two-dimensional with axial full-rotation symmetry)

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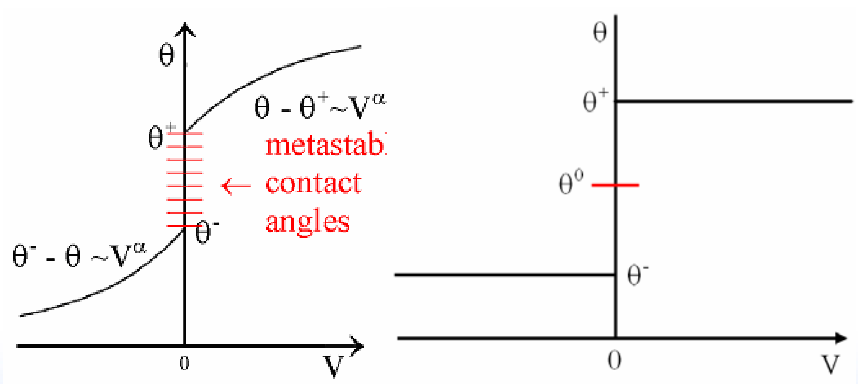

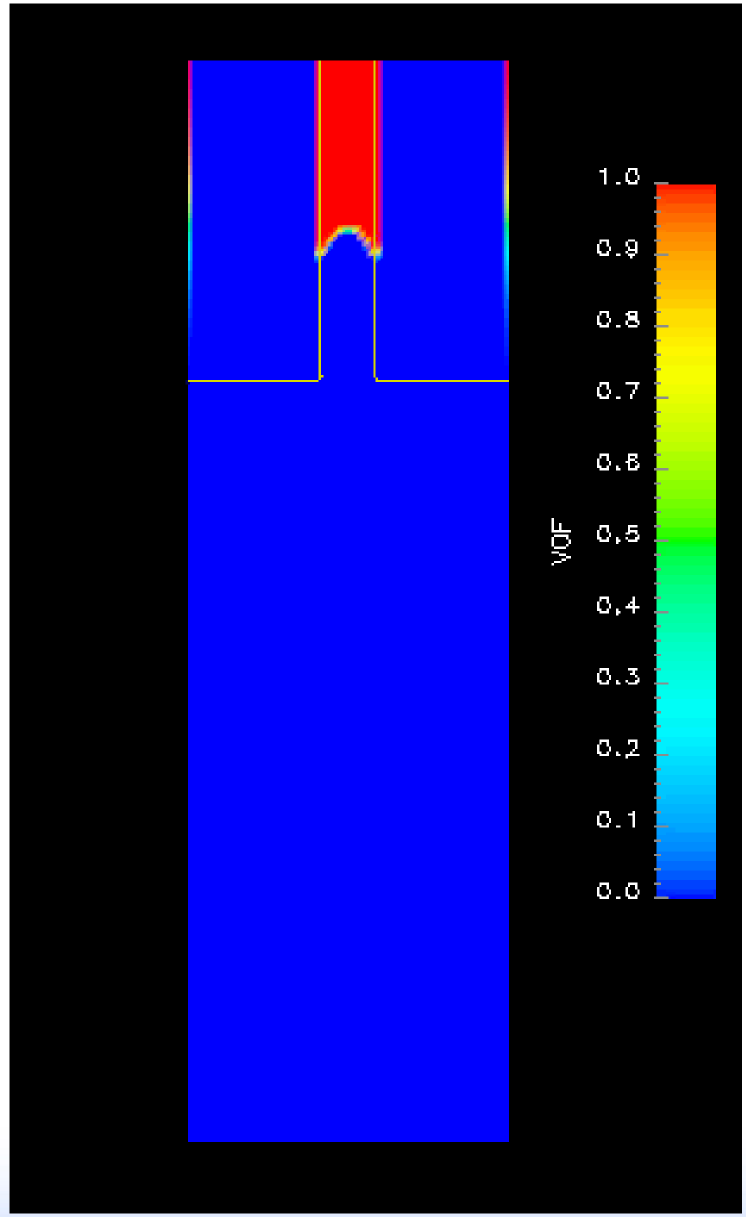

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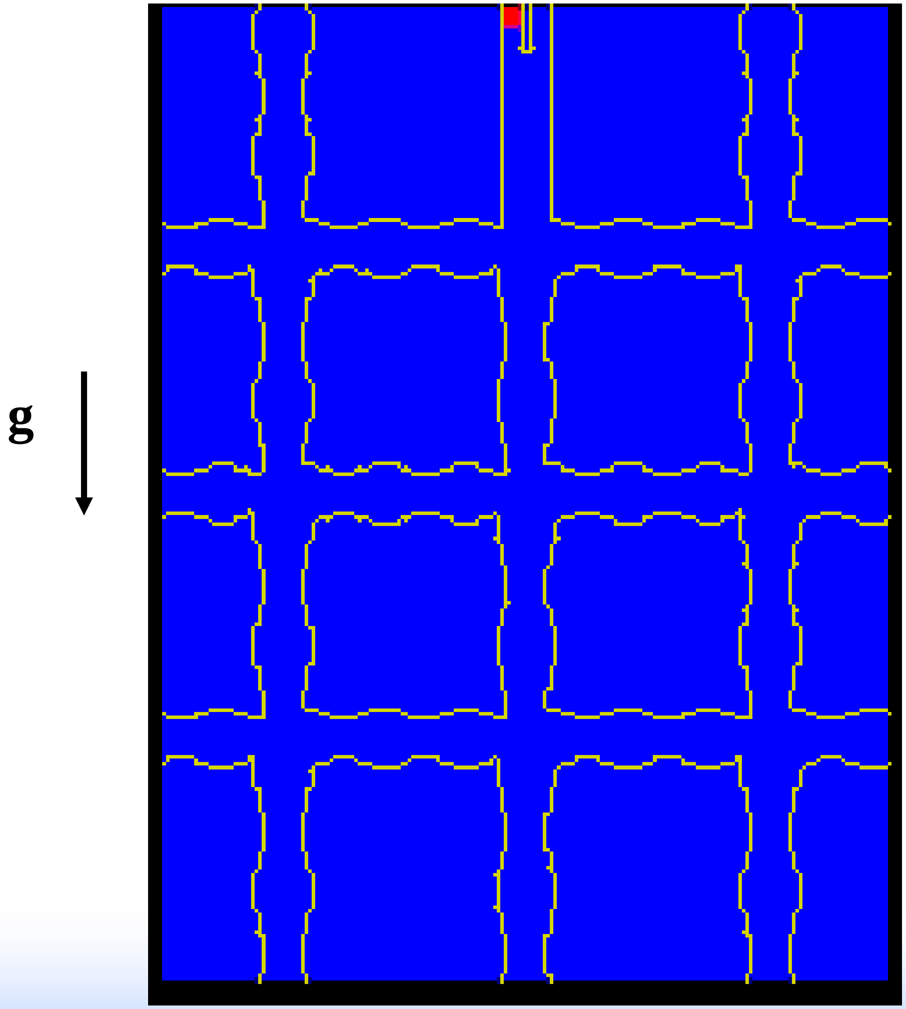
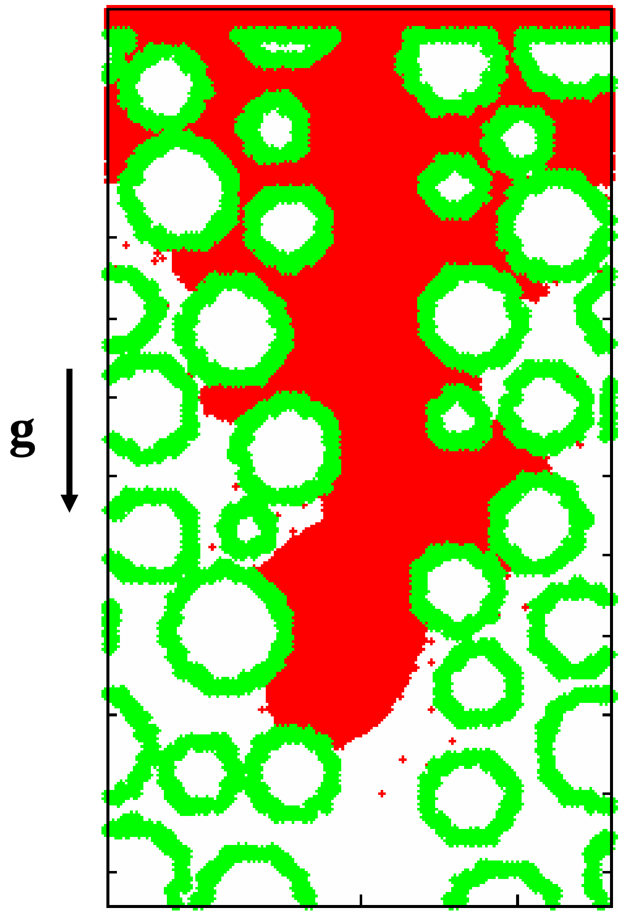
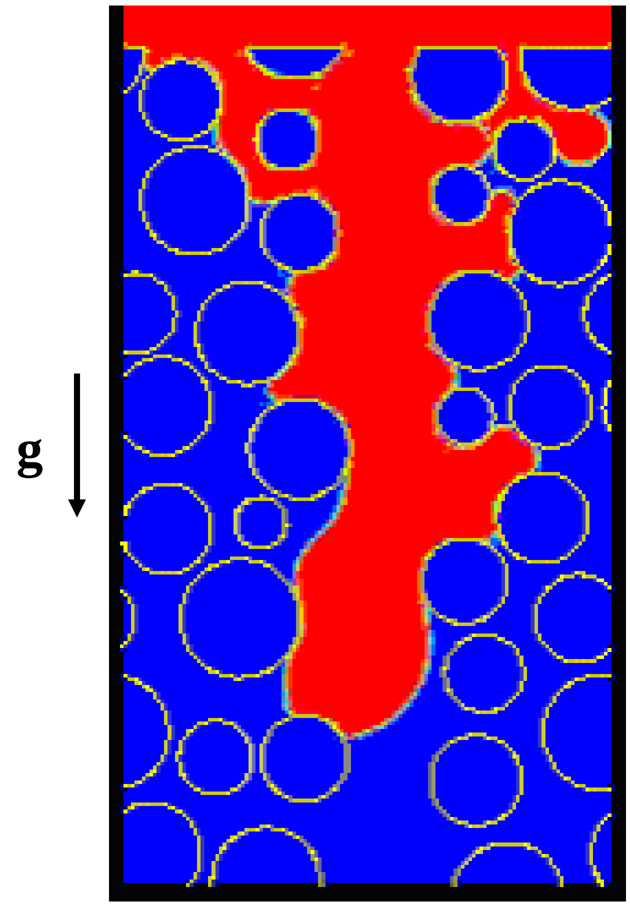
Simulation of multiphase fluid flow in fracture junction with VOF interface capturing



H. Huang, P.Meakin, and M. Liu, Geophysical Research Letters, **32:** L19402, doi:10.1029/2005GL023899. (2005)

Dissipative particle dynamics vs. grid-based simulation – penetration into fractured porous medium





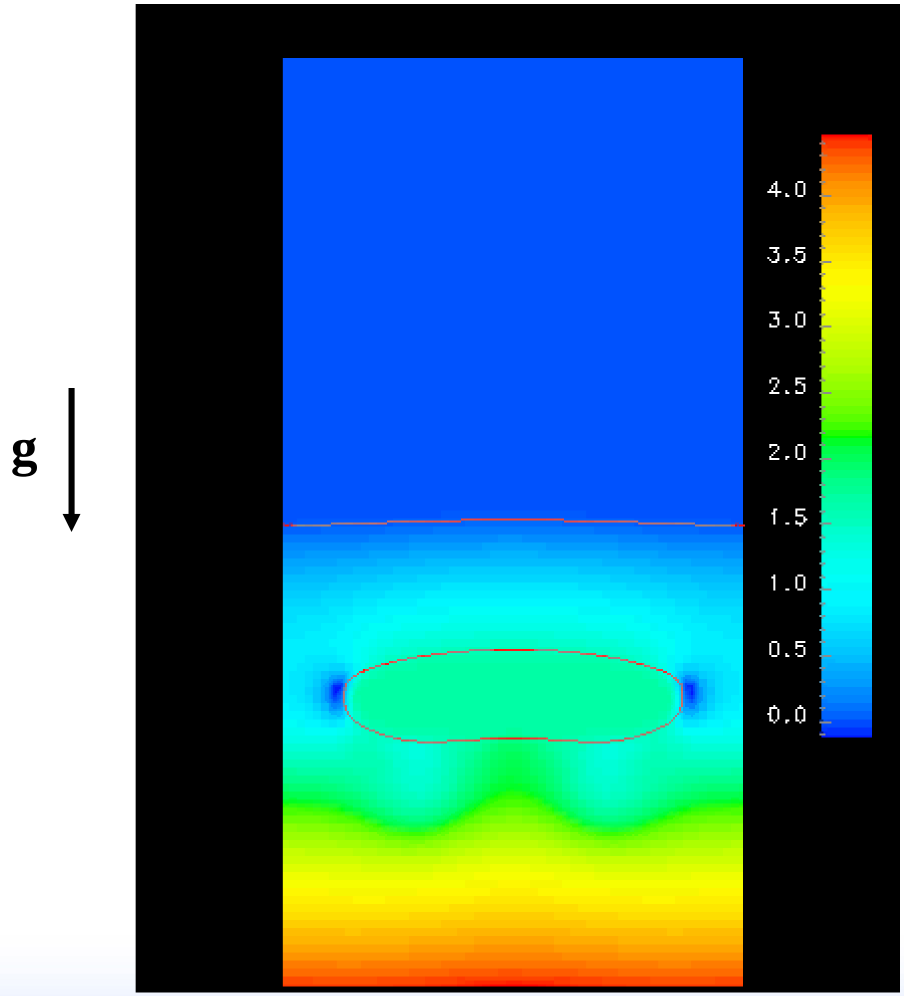
Finite volume -VOF

Level set interface capturing in combination with finite difference methods

- High computational efficiency
- Can handle large density and viscosity contrasts (water/air)
- Some mass loss: controllable
- Difficult to handle solid/water/air contact line dynamics: current challenge
- Most simple and elegant grid-based method for interface dynamics

Air bubble bursting near water surface – Level set interface tracking

Three-dimensional (two-dimensional with axial full-rotation symmetry)



Falling water droplet impacting on water surface – Level set interface tracking

Three-dimensional (two-dimensional with axial full-rotation symmetry)

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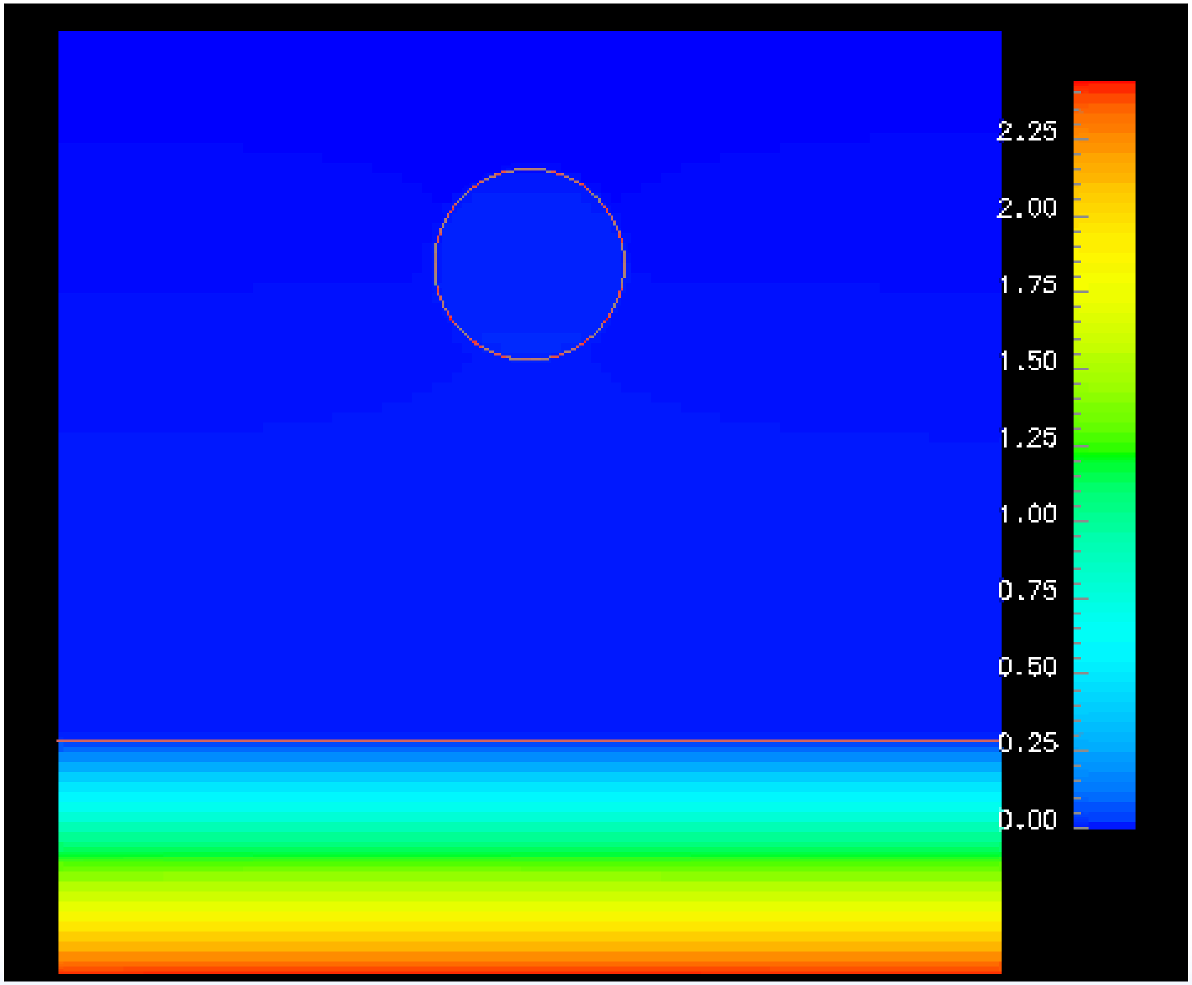
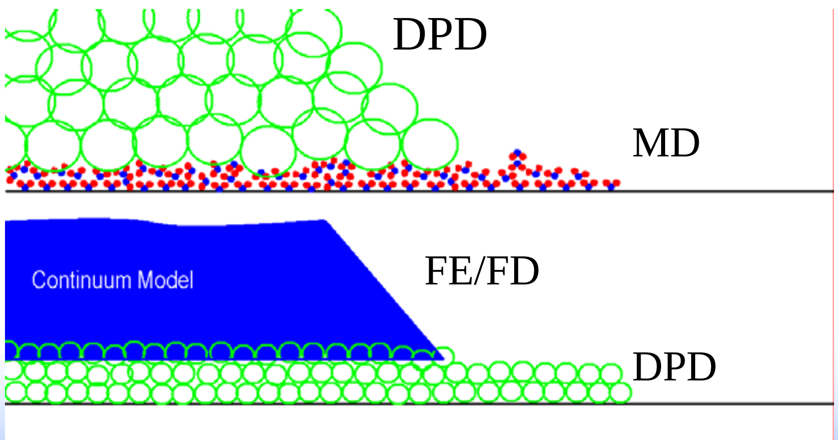


Going forward

- High performance computing (2-d →3-d)
- Hybrid particle/continuum multiscale modeling (use particle based model near interfaces and more computationally efficient grid-based continuum model in bulk)
- Multiscale simulations (particles of different sizes …)
- Better theory for particle-based models:
  - (relationship between particle-particle interactions, wetting behavior & fluid properties)
  - Spurious velocity fluctuations near interfaces
  - Theoretical foundation for multiscale modeling



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